

A Numerical Study of the Impacts of Volatile Component Blending on Diesel Spray Evaporation and Combustion

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Abstract

A multiphase computational fluid dynamics (CFD) code is used to simulate the evaporation and combustion processes of a diesel spray blended with a highly volatile component. The CFD code uses an Eulerian approach to model the liquid phase of diesel fuel with components of different boiling temperatures. The approach divides the droplets into size groups and assigns different boiling temperatures for each group. The CFD code accounts for liquid droplet flow, turbulent mixing, interfacial drag and heat transfer, droplet evaporation and combustion, radiation heat transfer, and pollutant kinetics. Using the code, a parametric study was conducted to investigate the impacts of a volatile component on the spray evaporation and combustion characteristics. The results indicate that the blending of a highly volatile component can have an impact on droplet evaporation rate and that thermal radiation is significant in spray combustion due to the formation of soot.

Introduction

Diesel spray combustion is one of the most active areas in engine researches. In a typical diesel spray process, liquid fuel is injected into a high-pressure chamber with hot gases. The liquid breaks up into a large number of droplets with various sizes. The droplets mix with the hot gases in the chamber and vaporize. Fuel vapor is burnt with the oxygen. The combustion process produces not only work but also pollutants, i.e., NO_x and unburnt hydrocarbons. There are several aspects that strongly affect the spray evaporation characteristics, subsequent combustion, and pollutant formation, and they have been the focus of many engine researches for a long period of time. Hiroyasu and Kadota [1] experimentally studied the injection of a diesel spray into a hot chamber and, using a liquid immersion technique, determined an empirical correlation for the droplet size distribution. Arail et al. [2] investigated in detail the fuel liquid disintegrating processes and showed that spray characteristics (e.g., spray tip penetration, break up length, spray angle) are strongly affected by operational and geometrical parameters such as inject velocity, inject and back pressure, nozzle length, etc. Wu et al. [3] experimentally studied the spray of water, n-hexane, and n-tetradecane and showed that spray angle depends strongly on gas and liquid density ratio, nozzle geometry, but only weakly on spray injection velocity. Tacuechi et al. [4] studied the atomization mechanism and temporal behavior of droplet size

distribution of a diesel spray and correlated experimental data to give droplet size distribution as a function of both space and time, demonstrating that diesel spray process can be very complicated. There are also studies on other aspects of diesel spray (i.e., effect of fuel viscosity and surface tension on Sauter Mean Diameter [5] and the effect of fuel flash point on spray evaporation and combustion [6].)

While experimental studies are the primary means in diesel engine researches, it suffers from the cost of expensive experimental apparatus and the infeasibility of detailed parametric studies. Numerical modeling, on the other hand, requires very little resources and has proved to be a viable and an effective approach in wide industrial applications. Examples include spray evaporation in various petroleum cracking units [7-9] and other combustion systems [10]. The complex phenomena of two-phase flow, turbulent heat and mass transfer, thermal radiation are governed by a set of differential equations derived from fundamental principles. Solutions to this set of differential equations can provide details of flow characteristics by its properties, e.g., pressure, temperature, velocity, species transport, etc.

Most numerical simulations in spray evaporation, combustion, and other related applications assumed that the liquid fuel has uniform thermal physical properties. Such an assumption has given fairly good numerical results in the past. Recently, people want to modify fuel's property by blending highly volatile

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components so that the blended fuel can burn more efficiently and produce less pollutant. Examples include the blending of oxygenates into diesel fuels. The blending of oxygenates is expected to change fuel's thermal physical properties, i.e., viscosity, surface tension, and boiling point. These changes will in turn affect the processes of spray evaporation, combustion, and pollutant formation. This study was conducted to make a preliminary assessment of the impacts of the blending of a highly volatile component on the diesel spray evaporation and combustion.

In this paper, the methodology and approach are introduced first, then the modeling of the spray with two boiling temperatures is described, and the results and discussion follow.

Methodology

Spray evaporation and combustion are complicated two-phase flow processes, involving turbulent heat and mass transfer, liquid droplets evaporation, chemical reactions, and radiation heat transfer. The behavior of these processes, however, can be described mathematically by a set of partial differential equations. The ICOMFLO code, developed at Argonne National Laboratory, is capable of simulating all of the interrelated phenomena. The code takes three steps to tackle the computation task. In first step, it computes a two-phase turbulent reacting flow by solving a set of nonlinear partial differential equations. During a spray combustion process, chemical reactions and species can be many, incorporation of a complete set of reaction equations and inclusion of all species into a CFD calculation are not only impractical but also causing severe numerical oscillations. ICOMFLO therefore lumps combustion species into four major ones (fuel, oxidizer, water vapor, and carbon dioxide) and replaces an Arrhenius type reaction model by one of integral type, which greatly enhances the code's numerical stability. In the second step, it calculates the formation and transport of combustion gaseous subspecies and soot, using pressure, temperature, density, and velocity fields from the reacting flow calculations. The subspecies under consideration include soot and CO, CO₂, H₂O, O₂, N₂, NO, and fuel. In the last step, it computes net radiation heat flux, using temperature and pressure fields from reacting flow calculation and subspecies and soot distributions from subspecies calculations. The net radiation heat flux is used as an additional source term in the enthalpy conservation equation of the reacting flow calculation. The whole computation process iterates through the three steps repeatedly until the calculation converges. The formulation details of subspecies, soot kinetics and radiation heat transfer computation are described in reference 11.

Formulations

A Cartesian coordinate system is chosen with the origin of the coordinate located at the center of the orifice (on the inlet plane) and the x-axis being parallel to the direction of the inlet flow. With this coordinate system and steady state assumption, the governing equations for the conservation of mass, momentum, energy, and species transport can be written in a common form as

$$\sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(\theta \rho u_i \xi - \Gamma_{\xi} \frac{\partial \xi}{\partial x_i} \right) = S_{\xi} \quad (1)$$

where, ξ , θ , x_i , and u_i are a general flow property, gas volume fraction, coordinates, and gas velocity components, respectively. Γ and S_{ξ} are the effective diffusivity and the sum of source terms for the general flow property ξ , respectively.

The fuel spray injection is considered through the orifice as a mixture of fuel vapor and droplets, and preheated air coming in from area outside the orifice. An Eulerian approach is adopted to describe the droplet flow. The approach discretizes an assumed inlet droplet size spectrum into a finite number of size groups. For each droplet size group, a set of governing equations for the conservation of mass, momentum, and energy can be derived and put in the following form

$$\sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(n_k u_{k,i} \xi - \Gamma_{\xi} \frac{\partial n_k \xi}{\partial x_i} \right) = S_{\xi}, \quad (2)$$

in which n_k is the droplet number density of size group k , $u_{k,i}$ ($i=1,2,3$) is the velocity component in the x_i direction of the k th droplet size group. Γ and S_{ξ} are the droplet diffusivity and the sum of source terms for the flow property ξ , respectively. Boundary conditions are that fluid neither slips at nor penetrates into chamber wall and that there are no normal fluxes for the temperature and species on the chamber wall. At the inlet plane conditions are specified for each variable, and no boundary condition is specified at the outlet plane, which can be justified when local Péclet number is sufficiently large [12].

Multi-Component Droplet Evaporation Model

ICOMFLO code employs phenomenon models to define effective diffusivities and source terms for each flow property in the corresponding governing equations. Major phenomenon models include an integral (as opposed to differential) reaction model, interfacial drag and heat transfer model, a modified turbulent k - ϵ model for a two phase flow, and a single

boiling point droplet evaporation model. Details of these models are described in references 7, 8, and 10.

An approach is developed to account for the vaporizing of a fuel droplet with two different boiling points. This approach can be used to efficiently model the evaporation of fuel spray with a different component. The droplets are divided into two groups, one comprising spherical droplets with one boiling point, the other with two boiling points. For a total of N size groups considered in the simulation, we assume that the smallest K (to be determined) groups possessing a uniform high boiling temperature T_h . The remaining $(N-K)$ large droplets group are having both boiling temperatures (T_h and T_l). In this way, after the volatile component vaporizes, the remaining droplet masses, from these large droplet groups, are reallocated to the small droplet groups, reflecting the droplet size shifting in an actual droplet vaporizing process. For a specific large droplet group j (with both T_h and T_l), we assume that the spherical droplet has an inner and outer part each with a uniform high and low boiling temperature, respectively, as shown in Figure 1.

When the droplet temperature reaches T_l the outer part of the sphere will evaporize (the corresponding mass m'_j will go into gas phase), and the remaining mass (Δm_j) will be allocated to the smaller size groups (e.g., size group i) with a higher boiling temperature.

$$m'_j = n_j \frac{4\pi}{3} (r_j^3 - r_i^3) \rho_l \quad (3)$$

and

$$\Delta m_j = m_j - m'_j = n_j \frac{4\pi}{3} r_i^3 \rho_l \quad (4)$$

where n_j is the droplet number density in j 's group and ρ_l is the liquid density.

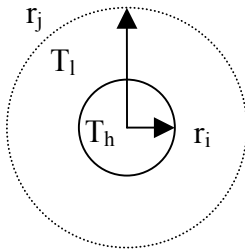


Figure 1. Schematic of a droplet possessing two boiling temperatures.

To determine how many groups that will possess both high and low boiling temperatures, we note that the summation of the volatile component masses from $(N-K)$ droplet size groups has to equal the total amount of volatile component in the fuel. We also note that the remaining high boiling point fuel can be

reallocated to several groups in the subgroup possessing high boiling point. In the present calculation, all of the remaining mass from large size groups is lumped into the largest droplet group in the subgroup that does not contain a volatile component. Due to the droplet mass reallocation, the droplet size distribution are effectively changed. As shown in Figure 2, droplet number densities in groups 8, 9, and 10 decreased, the number density in group 7 increased, and the rest of the spectrum remain unchanged.

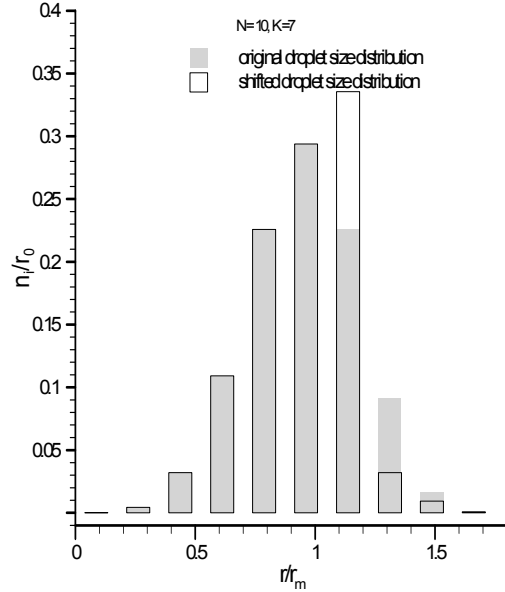


Figure 2. droplet size distribution for spray with single- and two-point boiling temperatures.

Numerical Approach

The set of governing equations mentioned above and the associated boundary conditions can be solved to obtain the velocity, pressure, density, temperature fields, and species concentrations. A control volume approach is used to discretize the the set of partial differential equations, the resulting set of nonlinear algebraic equation is solved iteratively using SIMPLE algorithm as described by Patankar [12]. In the present calculation, an iteration will be considered converged if the average mass residual of all cells is no greater than a prescribed convergence criterion, i.e., 10^{-10} . A typical converged result can be obtained in about 1500 iterations. Grid sensitivity (including number of droplet size groups) tests are performed to ensure that simulations will produce sufficiently accurate results and yet do not require excess computing resources.

Results and Discussion

The computational domain in our simulation is a three-dimensional chamber with 3 meters long and cross sectional area of 0.09 meters squared. Liquid fuel is injected into the chamber through the orifice (1 cm^2) on the left. Since the flow, temperature, species concentration fields are symmetric about the x-axis. We only show results in $z=0$ plane.

First we show the effect of multiple boiling points on individual droplet evaporations. We know that when droplet temperature reaches T_b , the volatile component in droplet will first vaporize and this will lead to a decrease in droplet mass (i.e., reduction of droplet number density.) The effect should results in decreases in droplet number density in large droplet groups (e.g., groups 8-10.) The result is demonstrated in Figure 3, which plots the droplet number density of the group 8. The results computed with a single component model (Fig. 3a) are compared with those with the new multi-component model (Fig. 3b). The droplets in Fig 3b vaporize much faster than those in Fig. 3a. However, for a smaller droplet groups, the impact on the evaporation is much less. Figure 4 shows the average axial fuel vapor flow rate. As can be seen from the figure that the fuel vapor flow rate (solid line) near the inlet plane increases due to the quick vaporizing of the volatile component. In the later part of the process, the flow rate is smaller than the unblended case (dash dotted line) is due to the fact that the total masses in the two cases are the same (i.e., area under the two curves has to be the same.)

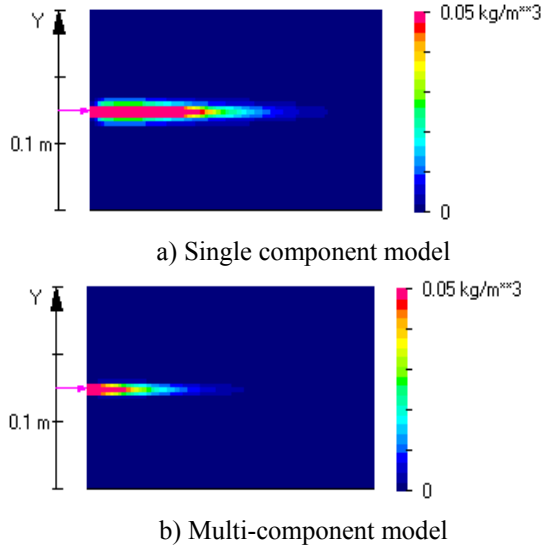


Figure 3. Group 8 Droplet Number Densities

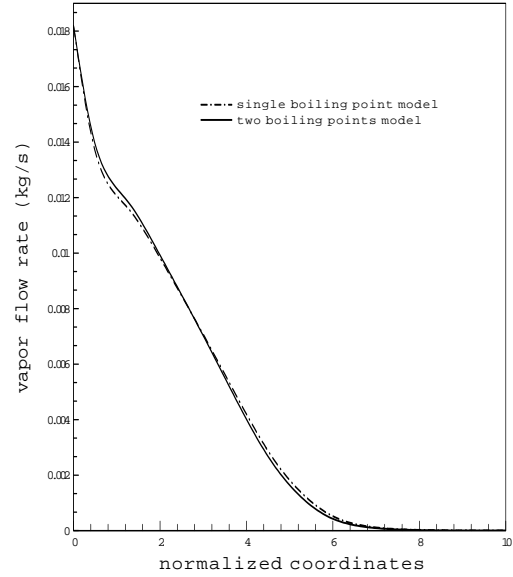


Figure 4. Axial fuel vapor flow rate.

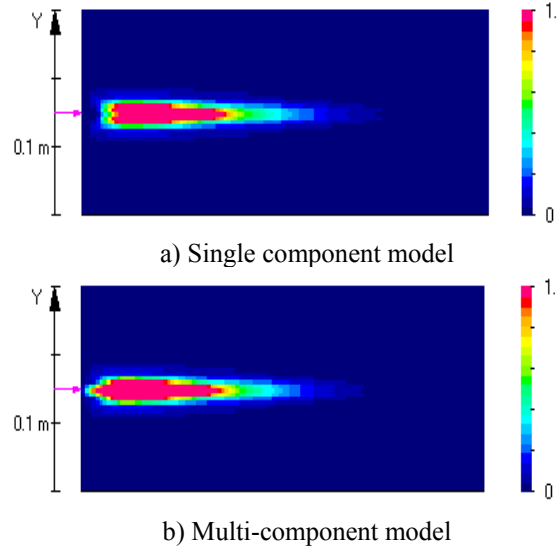


Figure 5. Overall Evaporation Rate

In Figure 5, the overall droplet evaporation rate is shown. As can be seen from the figure, there are noticeable differences in vaporizing rates near the injector location. In the case of droplet vaporizing with two boiling points (figure 5b), it can be seen that with a volatile component in the droplet, it takes less time (a shorter distance from the inlet) for droplets to heat up and vaporize, consequently, the evaporation rate of droplet in a small area near the orifice much higher. The contribution to this increase in evaporation rate clearly comes from the quick vaporizing of volatile component in large size droplet. This result is in consistent with that in Figure 3. The later stage of

evaporation of the two cases is almost identical. This is expected from our model, since after a volatile component vaporizes the remaining droplet is unchanged.

Figure 6 shows the distribution of carbon dioxide in the combustion chamber. As can be seen from the figure, there are some differences in carbon dioxide distribution in the center of the chamber. The model predicts slightly higher maximum carbon dioxide mass fraction value for the combustion of fuels with a volatile component. This small difference could be attributable to the slightly higher axial fuel vapor flow rate when a volatile component is present.

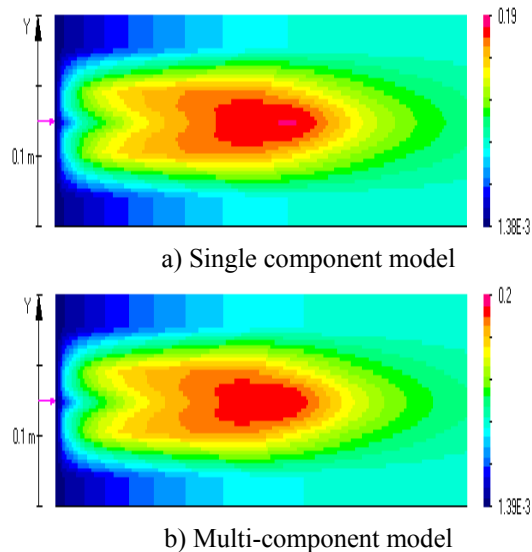


Figure 6. Distribution of carbon dioxide

Figure 7 shows the radiation emissive flux in the combustion chamber. The result shows that most emission concentrates in the central core of the chamber. This can be explained in connection with the soot distributions. Soot generally forms in fuel rich regions and plays an important role in thermal radiation. In the current simulation, soot is highly confined to a local region in the center of the chamber (not shown). One reason for this distribution is that relatively high level of oxygen in the air encompasses the fuel vapor region so that most of soot gets oxidized when it diffuses to the outer region of the chamber. Compared to the evaporation of individual droplets, the effect of multiple boiling temperatures on soot formation is only.

Figure 8 presents the gas phase temperature distribution in the combustion chamber without (a) and with (b) thermal radiation accounted for. It can be easily seen that radiation not only significantly modified the gas temperature distribution it also reduced the highest flame temperature by 102 degree

Kelvin. This difference could have a significant impact in predicting the pollutant formation in the combustion zone.

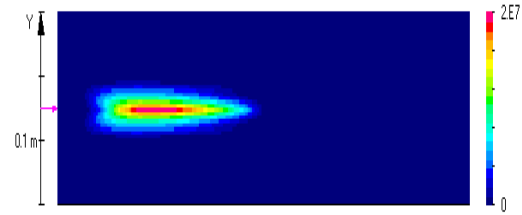


Figure 7 Radiation Emissive Fluxes.

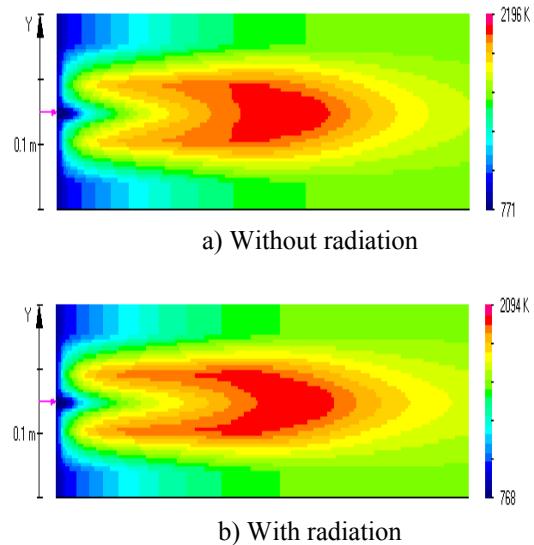


Figure 8 Temperature Distributions

Conclusion

In this study, the effect of a volatile component on fuel droplet evaporation and combustion was investigated. A new approach to model the droplet evaporation with two different boiling temperatures was developed. The model has been incorporated into the CFD code and validated by its results that capture the physics of droplet evaporation. The results show that multiple boiling temperatures have significant effect on individual droplet vaporizing and noticeable effect on overall evaporation characteristics. Considering the possible effect of volatile components on other physical properties (e.g., viscosity and surface tension) of fuel droplet, blending volatile components into a fuel could have significant effects on fuel droplet evaporation, combustion, and pollutant formation. The results also show that inclusion of thermal radiation calculation in CFD modeling of spray combustion is necessary for accurate description of temperature in the flame.

Acknowledgement

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